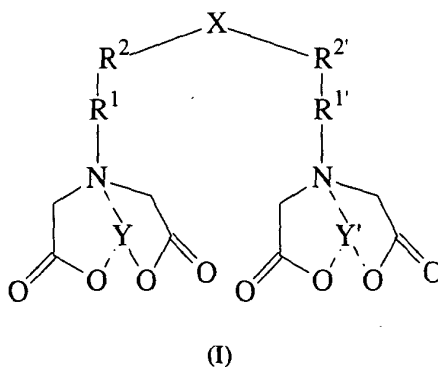


WE CLAIM:

1. A molecule for labeling a target material, comprising:
a conjugate of a transition metal compound with a detectable group, said conjugate having the general structural formula (I), and tautomers, salts, and acids thereof:

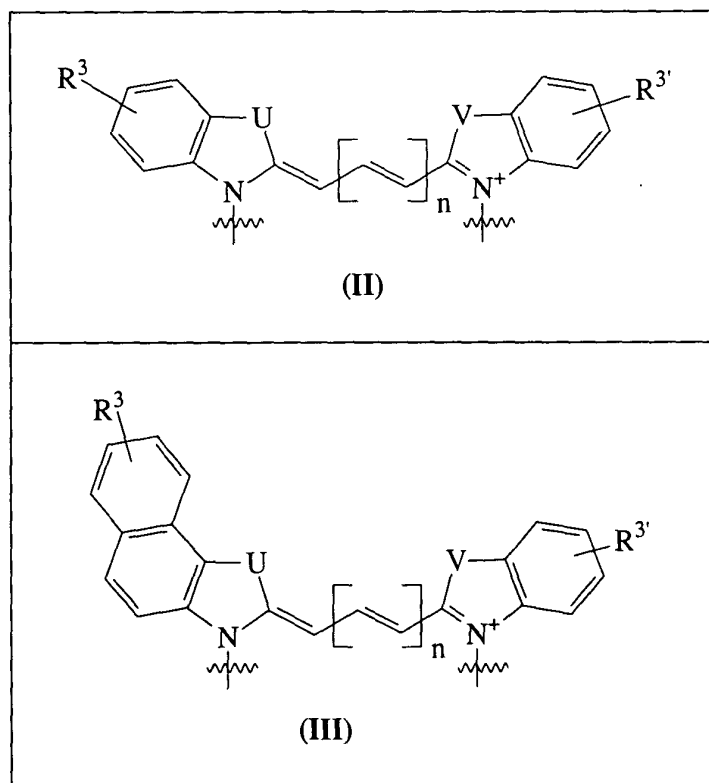


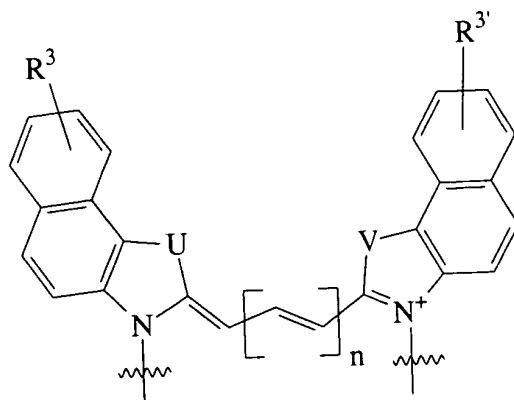
wherein (a) Y and Y' are each a transition metal; (b) R¹ and R^{1'} are each independently CH(COO⁻), CH(COOH), or absent; (c) R² and R^{2'} are linear or branched, optionally substituted, linkers of from about 3.0 to about 20 Å long; and (d) X is a detectable group.

2. The molecule according to claim 1, wherein (R¹ + R²) and (R^{1'} + R^{2'}) are each independently linkers of from about 3.0 Å to about 15 Å long, with the proviso that the difference in length between (R¹ + R²) and (R^{1'} + R^{2'}) is less than or equal to about 6 Å.
3. The molecule according to claim 2, wherein the length of (R¹ + R²) is equal to the length of (R^{1'} + R^{2'}).
4. The molecule according to claim 1, wherein Y and Y' are each independently selected from the group consisting of Ni²⁺, Co²⁺, Cu²⁺, and Zn²⁺.
5. The molecule according to claim 4, wherein Y and Y' are each Ni²⁺.

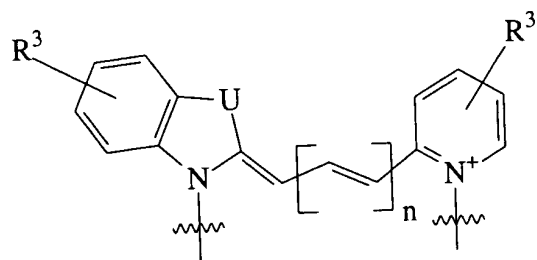
744-37 PCT/US/CIP I

6. The molecule according to claim 1, wherein the detectable group is selected from the group consisting of a fluorescent moiety, a phosphorescent moiety, a luminescent moiety, an absorbent moiety, a photosensitizer, a spin label, a radioisotope, an isotope detectable by nuclear magnetic resonance, a paramagnetic atom, a heavy atom, a hapten, a crosslinking agent, a cleavage agent, and combinations thereof.
7. The molecule according to claim 1, wherein X is a fluorescent moiety.
8. The molecule according to claim 1, wherein X is derived from a cyanine dye.
9. The molecule according to claim 1, wherein X is derived from a squaraine dye.
10. The molecule according to claim 1, where X is selected from the group consisting of:

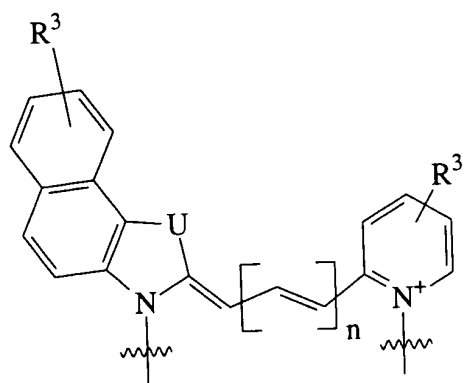




(IV)



(V)

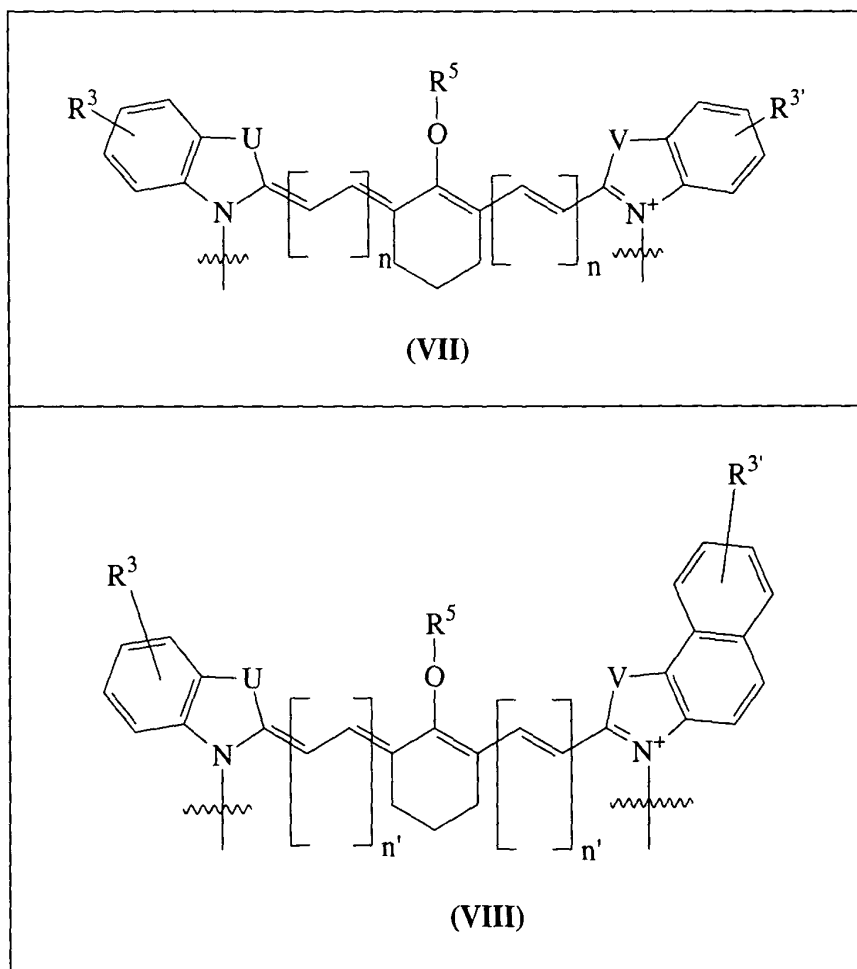


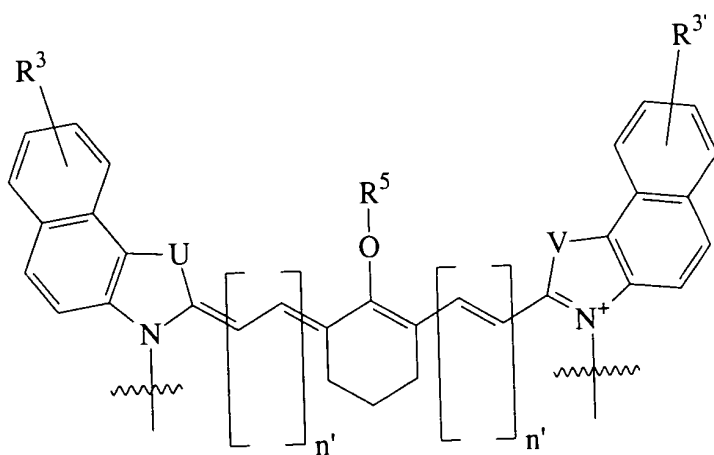
(VI)

wherein (a) U and V are each independently $C(R^4)_2$, NH, O, S, or $(CH_2)_2$; (b) R^3 and $R^{3'}$ are each independently H or sulfonate; (c) R^4 is H, CH_3 , CH_2CH_3 , or $(CH_2)_2CH_3$; and (d) n is 0 or an integer of from 1 to 6.

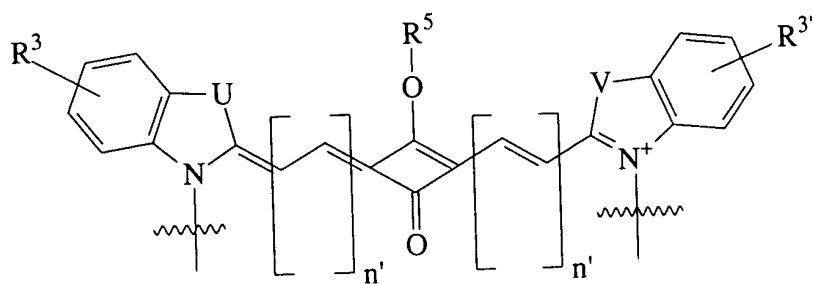
744-37 PCT/US/CIP I

11. The molecule according to claim 10, wherein n is 1, 2 or 3.
12. The molecule according to claim 1, where X is selected from the group consisting of:

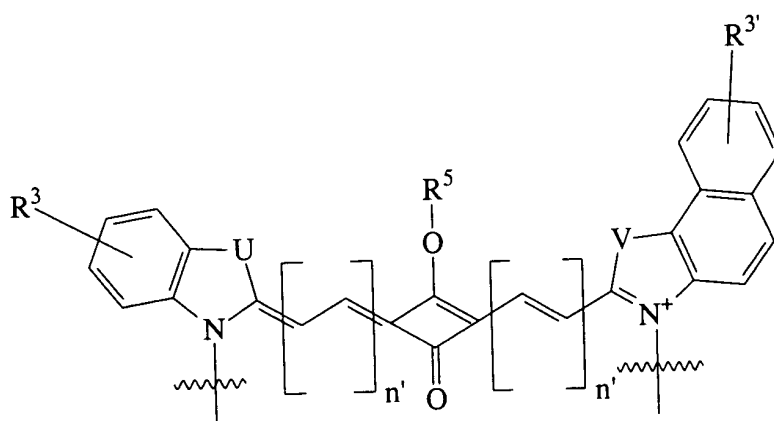




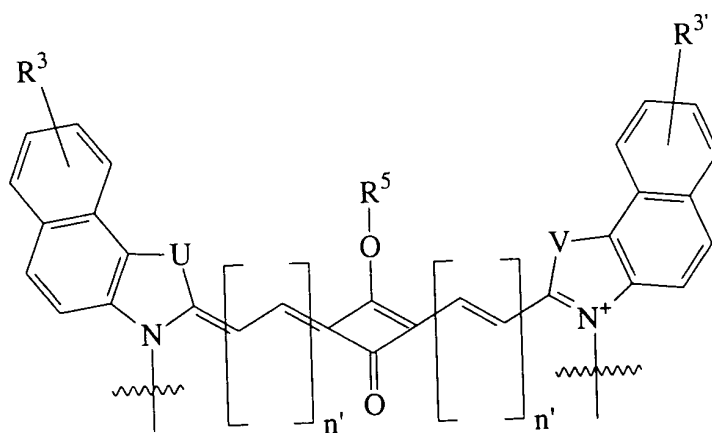
(IX)



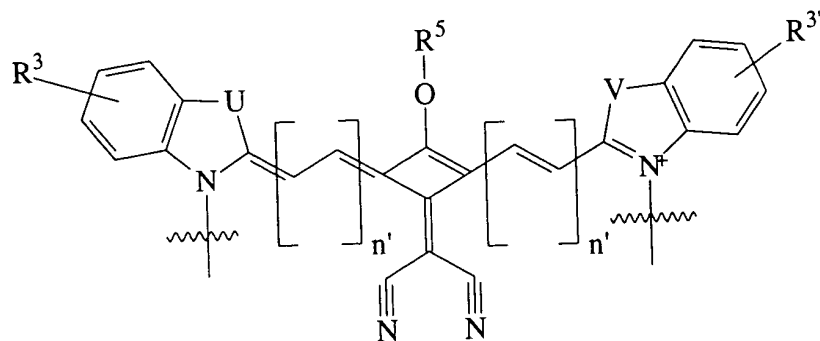
(X)



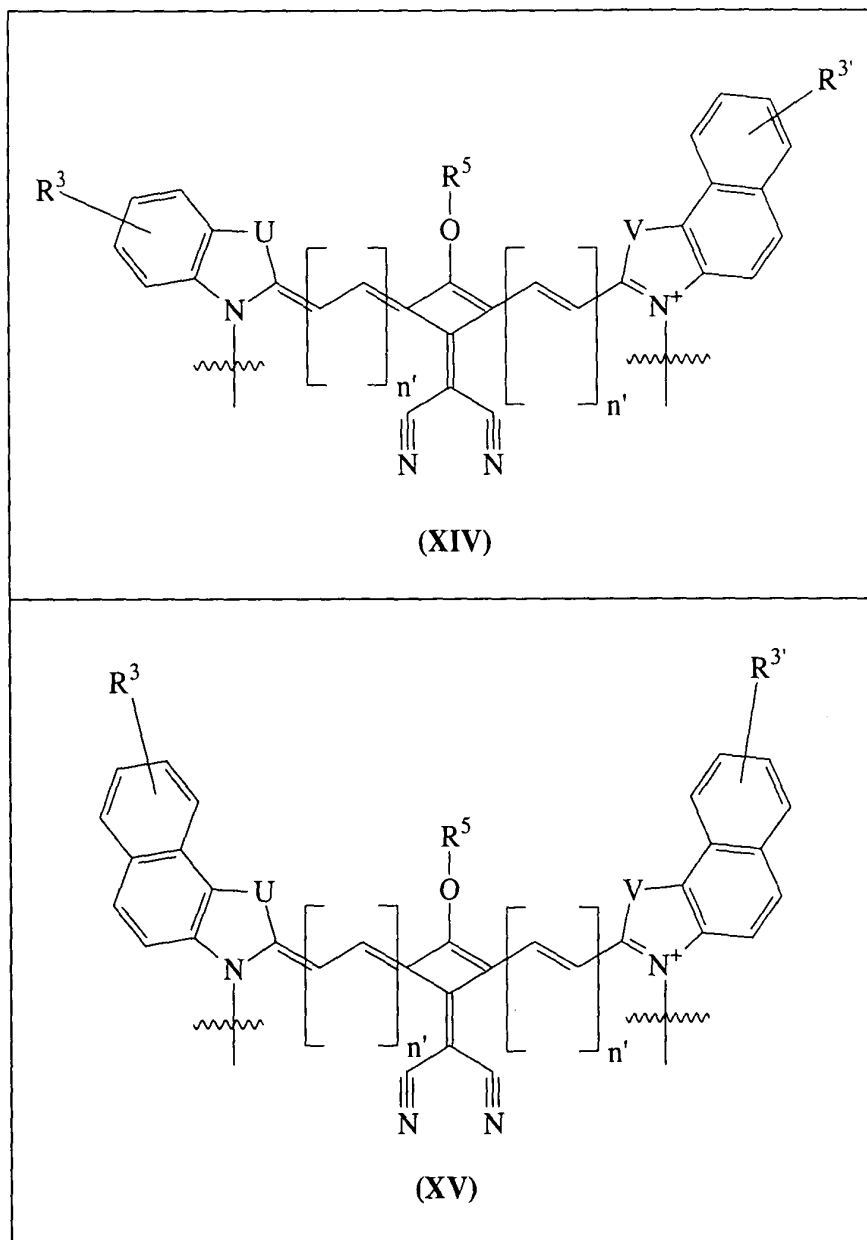
(XI)



(XII)



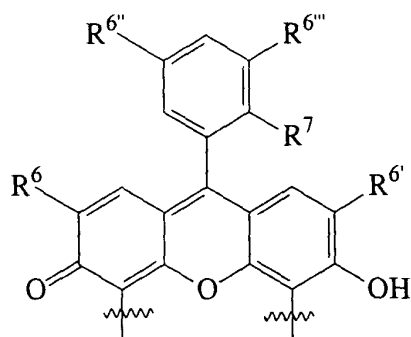
(XIII)



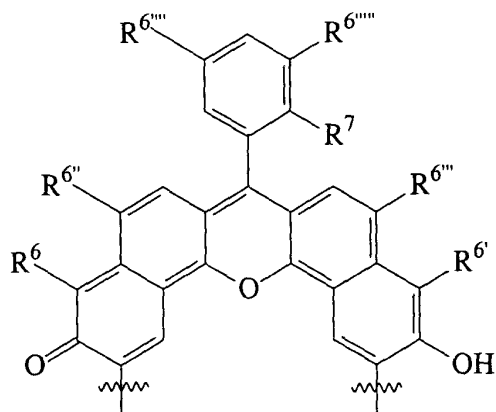
wherein (a) U and V are each independently $\text{C}(\text{R}^4)_2$, NH, O, S, or $(\text{CH}_2)_2$; (b) R^3 and $\text{R}^{3'}$ are each independently H or sulfonate; (c) R^4 is H, CH_3 , CH_2CH_3 , or $(\text{CH}_2)_2\text{CH}_3$; (d) R^5 is absent or is selected from the group consisting of H, an alkyl group, and an aryl group; and (e) n' is 0 or an integer of from 1 to 3.

13. The molecule according to claim 12, wherein n is 0, 1, or 2.

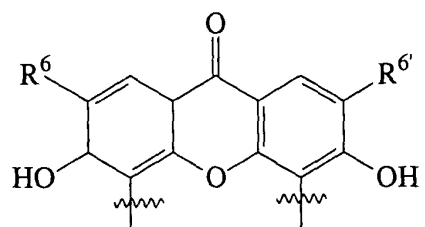
14. The molecule according to claim 1, where X is selected from the group consisting of:



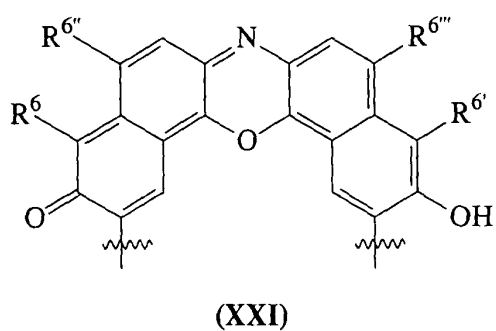
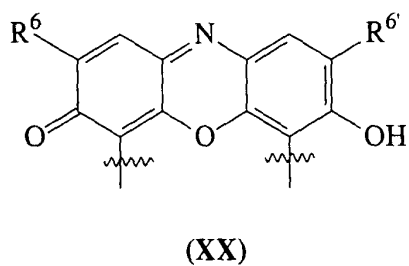
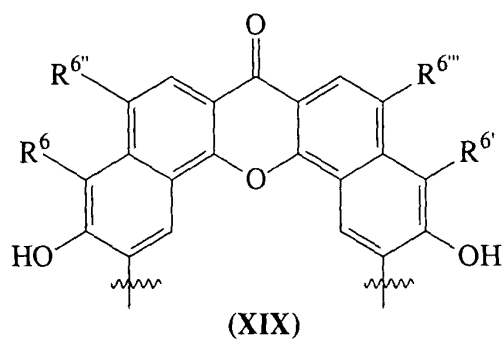
(XVI)



(XVII)



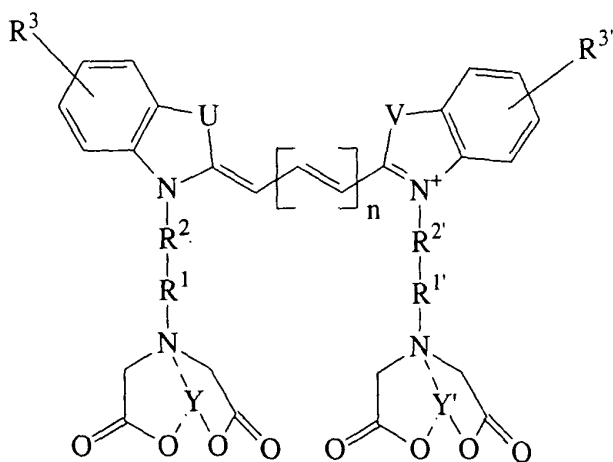
(XVIII)



wherein (a) R^6 , $R^{6'}$, $R^{6''}$, $R^{6'''}$, $R^{6''''}$, and $R^{6''''}$ are each independently hydrogen, halogen, hydroxyl, or alkoxyl; and (b) R^7 , when present, is hydrogen, carboxyl, carboxylate or sulfonate.

15. The molecule according to claim 1, wherein said molecule is capable of traversing a biological membrane.

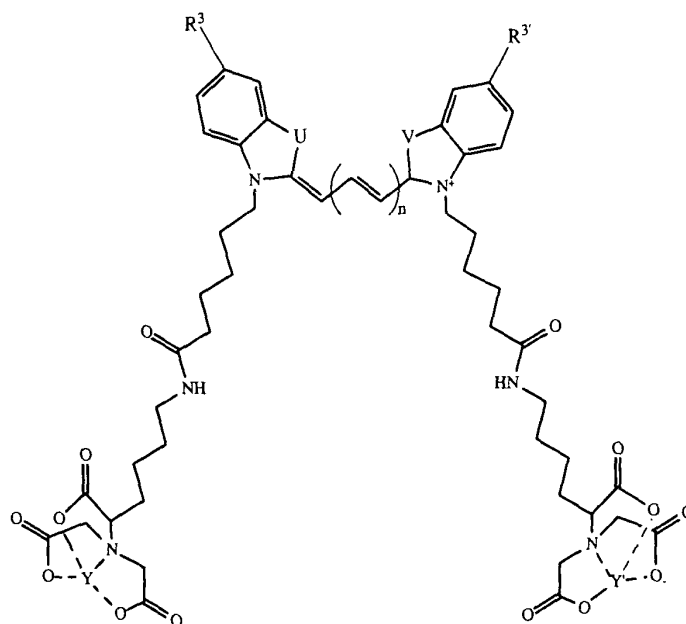
16. A molecule having two pendant transition-metal-chelate moieties according to the general structural formula:



(XXII)

wherein (a) Y and Y' are each a transition metal; (b) U and V are each independently $C(R^4)_2$, NH, O, S, or $(CH)_2$; (c) R^1 and $R^{1'}$ are each independently $CH(COO^-)$, $CH(COOH)$, or absent; (d) R^2 and $R^{2'}$ are each independently linear or branched, optionally substituted, linkers of from about 3.0 to about 20 Å long; (e) R^3 and $R^{3'}$ are each independently H or sulfonate; (f) R^4 is H, CH_3 , CH_2CH_3 , or $(CH_2)_2CH_3$; and (g) n is 0 or an integer of from 1 to 6.

17. The molecule according to claim 16, wherein $(R^1 + R^2)$ and $(R^{1'} + R^{2'})$ are each independently linkers of from about 3.0 Å to about 15 Å long, with the proviso that the difference in length between $(R^1 + R^2)$ and $(R^{1'} + R^{2'})$ is less than or equal to about 6 Å.
18. The molecule according to claim 16, wherein Y and Y' are each independently selected from the group consisting of Ni^{2+} , Co^{2+} , Cu^{2+} , and Zn^{2+} .
19. The molecule according to claim 16, wherein Y and Y' are each Ni^{2+} .
20. The molecule according to claim 16, wherein n is 1, 2, or 3.
21. A molecule with two pendant transition-metal-chelate moieties according to general structural formula:



(XXIII)

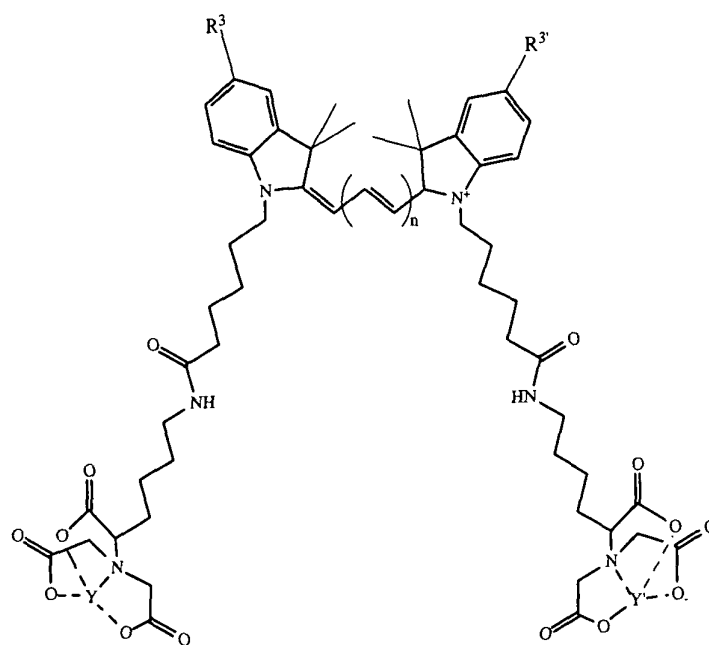
wherein (a) Y and Y' are each a transition metal; (b) U and V are each independently $C(R^4)_2$, NH, O, S, or $(CH)_2$; n is 0 or an integer of from 1 to 6; (c) R^3 and $R^{3'}$ are each independently H or sulfonate; (e) R^4 is H, CH_3 , CH_2CH_3 , or $(CH_2)_2CH_3$; and (f) n is 0 or an integer of from 1 to 6.

22. The molecule according to claim 21, wherein Y and Y' are each independently selected from the group consisting of Ni^{2+} , Co^{2+} , Cu^{2+} , and Zn^{2+} .

23. The molecule according to claim 21, wherein Y and Y' are each Ni^{2+} .

24. The molecule according to claim 21, wherein n is 1, 2, or 3.

25. A molecule with two pendant transition-metal-chelate moieties according to general structural formula:



(XXIV)

wherein Y and Y' are each a transition metal; R^3 and $R^{3'}$ are each independently H or sulfonate; and n is 1, 2, 3, or 4.

26. The molecule according to claim 25, wherein Y and Y' are each independently selected from the group consisting of Ni^{2+} , Co^{2+} , Cu^{2+} , and Zn^{2+} .

27. The molecule according to claim 25, wherein Y and Y' are each Ni^{2+} .

28. The molecule according to claim 25, wherein n is 1, 2, or 3.

29. A method for imparting detectable properties to at least one target material, the method comprising the step of reacting:

(a) a target material having a target sequence comprising an amino acid sequence of the form: $(H)_i$ wherein H is histidine, and i is an integer of from 4 to 12; and

(b) at least one molecule according to Formula (I) under conditions sufficient to permit transition-metal-chelate moieties of said molecule to associate with said target sequence.

744-37 PCT/US/CIP I

30. The method according to claim 29, wherein said target material is a polypeptide.
31. The method according to claim 29, wherein said target sequence is SEQ ID NO. 3.
32. A method for detecting at least one target material of interest, said method comprising:
 - (a) providing a target material containing a target sequence, said target sequence comprising an amino acid sequence of the form: (H)_i wherein H is histidine, and i is an integer of from 4 to 12;
 - (b) incubating said target material with at least one molecule according to Formula (I) having a detectable group, for a time period sufficient to allow labeling of said target material; and
 - (c) detecting said detectable group, thereby detecting said target material.
33. The method according to claim 32, wherein said target material is located within a material selected from the group consisting of a cuvette, a microtiter plate, a capillary, a flow cell, a test tube, a gel, a blot and a biological sample.
34. The method according to claim 32, wherein said target material is a polypeptide.
35. The method according to claim 32, wherein step (b) is performed in a gel matrix.
36. The method according to claim 32, wherein step (b) is performed in a complex mixture of components.
37. The method according to claim 32, wherein labeled target material is separated from other components following step (b).
38. The method according to claim 32, wherein labeled target material is not separated from other components following step (b).
39. The method according to claim 32, wherein said detectable group is a fluorescent moiety.

744-37 PCT/US/CIP I

40. The method according to claim 32, wherein said detecting step includes detecting a fluorescence property.
41. The method according to claim 40, wherein said fluorescence property is at least one of a fluorescence-emission intensity, a fluorescence lifetime, a fluorescence anisotropy, a fluorescence polarization, and a fluorescence correlation.
42. A method for determining the localization, concentration, or interactions of at least one target material of interest on or within a cell, tissue, organ, or organism, comprising the steps of:
- (a) providing a cell, tissue, organ, or organism containing a target material containing a target sequence, said target sequence comprising an amino acid sequence of the form: $(H)_i$ wherein H is histidine, and i is an integer of from 4 to 12;
 - (b) incubating said cell, tissue, organ, or organism with a molecule according to Formula (I) having a detectable group, for a time period sufficient to allow labeling of said target material; and
 - (c) detecting said detectable group, thereby determining the localization, concentration, or interactions of said target material.
43. The method according to claim 42, wherein said target material is a polypeptide.
44. The method according to claim 42, wherein said detectable group is a fluorescent moiety.
45. The method according to claim 42, wherein said detecting step includes detecting a fluorescence property.
46. The method according to claim 45, wherein said fluorescence property is at least one of a fluorescence-emission intensity, a fluorescence lifetime, a fluorescence anisotropy, a fluorescence polarization, and a fluorescence correlation.

744-37 PCT/US/CIP I

47. An assay method for monitoring a binding process comprising the steps of:
- (a) reacting a first component of a specific binding pair with a second component of said pair, with said first component being labeled with a molecule according to Formula (I) having a detectable group; and
 - (b) monitoring said reaction by monitoring a change in a signal of said detectable group.
48. An assay method for monitoring a binding process, comprising the steps of:
- (a) reacting a first component of a specific binding pair with a second component of said pair, with said first component being labeled with a molecule according to Formula (I) having a detectable group; and
 - (b) monitoring said reaction by monitoring at least one of a fluorescence-emission intensity, a fluorescence lifetime, a fluorescence anisotropy, a fluorescence polarization, and a fluorescence correlation of said detectable group.
49. An assay method for monitoring a binding process comprising the steps of:
- (a) reacting a first component of a specific binding pair with a second component of said pair, with said first component being labeled with a molecule according to Formula (I) wherein X of Formula (I) is a fluorochrome, and said second component including Z, wherein Z is capable of participating in fluorescence energy transfer, fluorescence quenching or exciton formation with X and is selected from the group including a fluorochrome and chromophore; and
 - (b) monitoring said reaction by monitoring fluorescence of X.
50. An assay method for monitoring a binding process comprising the steps of:
- (a) reacting a first component of a specific binding pair with a second component of said pair, with said first component being labeled with a molecule according to Formula (I) wherein X of Formula (I) is selected from the group consisting of a fluorochrome and a chromophore, and said second component including Z, wherein Z is a fluorochrome able to participate in fluorescence energy transfer, fluorescence quenching, or exciton formation with X; and
 - (b) monitoring the reaction by monitoring fluorescence of Z.

744-37 PCT/US/CIP I

51. An assay method for monitoring a reaction, comprising the steps of:
- (a) reacting a first analyte with a second analyte, said first analyte being labeled with a molecule according to formula (I) having a detectable group; and
 - (b) monitoring said reaction by monitoring a change in a detectable property of said detectable group.
52. The method according to claim 51, wherein said reaction is selected from the group consisting of a protein-protein binding event, a protein-self-association event, a protein-protein cleavage event, and a conformational change of a protein.
53. A method for isolating at least one target material of interest comprising:
- (a) contacting at least one molecule according to Formula (I) immobilized on a solid support, with a solution containing a target material having a target sequence of the form: $(H)_i$ wherein H is histidine, and i is an integer of from 4 to 12, under conditions that allow binding of said polypeptide to said immobilized molecule of Formula (I); and
 - (b) eluting said target material with a low-molecular weight monothiol or low-molecular-weight dithiol.
54. The method according to claim 53, further comprising the step of washing said solid support to remove unbound material before eluting said target material.
55. The method according to claim 53, wherein said solid support is selected from the group consisting of a surface, a bead, a gel, and a chromatographic matrix.
56. A method for immobilizing at least one target material of interest including:
- (a) contacting at least one molecule according to Formula (I) immobilized on a solid support with a solution containing a target material having a target sequence of the form: $(H)_i$ wherein H is histidine, and i is an integer of from 4 to 12, under conditions that allow binding of said target material to said immobilized molecule of Formula (I).

744-37 PCT/US/CIP I

57. The method of claim 56, further comprising the step of washing said solid support to remove unbound material.
58. The method according to claim 56, wherein said solid support is selected from the group consisting of a surface, a bead, a gel, and a chromatographic matrix.
59. A kit, comprising:
- (a) a molecule according to Formula (I); and
 - (b) a molecule including a target sequence, said target sequence comprising an amino acid sequence of the form: $(H)_i$ wherein H is histidine, and i is an integer of from 4 to 12.
60. A kit comprising:
- (a) a molecule according to formula (I); and
 - (b) a reagent that promotes the formation of a complex between the molecule according to formula (I) and a target sequence, said target sequence comprising an amino acid sequence of the form: $(H)_i$ wherein H is histidine, and i is an integer of from 4 to 12.
61. The method of synthesis of a compound of claim 1 by coupling:
- (a) a synthon consisting of a bis-activated-ester derivative of a detectable group; and
 - (b) a synthon consisting of an amine or hydrazide derivative of a chelator;
- and then adding a transition metal.
62. The method of claim 61, wherein said chelator is protected during said coupling and deprotected thereafter.
63. The method of synthesis of a compound of claim 1 by coupling:
- (a) a synthon selected from mono-chelator-functionalized 2,3,3-trimethylindole, mono-chelator-functionalized 2,3,3-trimethylbenzindole, mono-chelator-functionalized 2-methylpyridine, mono-chelator-functionalized 2-methyl-benzothiazole, mono-chelator-functionalized 2-methyl-naphthothiazole, mono-chelator-functionalized 2-methyl-benzoxazole, and mono-chelator-functionalized 2-methyl-naphthoxazole;

744-37 PCT/US/CIP I

(b) a synthon, identical or nonidentical to the synthon in (a), selected from the group in (a); and

(c) a synthon containing at least one carbon atom;
and then adding a transition metal.

64. The method of claim 63, wherein said coupling is performed as a single reaction step.

65. The method of claim 63, wherein said coupling comprises: either (i) first reacting (a) and (c) to form a product, followed by further reacting the product with (b); or (ii) first reacting (b) and (c) to form a product, followed by further reacting the product with (a).

66. The method of claim 63, wherein said chelator is protected during said coupling and deprotected thereafter.

67. The method of synthesis of a compound of claim 1 by coupling:

(a) a synthon selected from mono-chelator-functionalized 2,3,3-trimethyl-5-sulfonato-indole, mono-chelator-functionalized 2,3,3-trimethyl-6-sulfonato-benzindole, mono-chelator-functionalized 2-methyl-5-sulfonato-pyridine, mono-chelator-functionalized 2-methyl-5-sulfonato-benzothiazole, mono-chelator-functionalized 2-methyl-6-sulfonato-naphthothiazole, mono-chelator-functionalized 2-methyl-5-sulfonato-benzoxazole, and mono-chelator-6-sulfonato-functionalized 2-methyl-naphthoxazole;

(b) a synthon, identical or nonidentical to the synthon in (a), selected from the group in (a); and

(c) a synthon containing at least one carbon atom;
and then adding a transition metal.

68. The method of claim 67, wherein said coupling is performed as a single reaction step.

69. The method of claim 67, wherein said coupling comprises: either (i) first reacting (a) and (c) to form a product, followed by further reacting the product with (b); or (ii) first reacting (b) and (c) to form a product, followed by further reacting the product with (a).

744-37 PCT/US/CIP I

70. The method of claim 67, wherein said chelator is protected during said coupling and deprotected thereafter.

71. The method of synthesis a compound of claim 1 by coupling:

(a) a synthon selected from mono-chelator-functionalized 2,3,3-trimethylindole, mono-chelator-functionalized 2,3,3-trimethylbenzindole, mono-chelator-functionalized 2-methyl-pyridine, mono-chelator-functionalized 2-methyl-benzothiazole, mono-chelator-functionalized 2-methyl-naphthothiazole, mono-chelator-functionalized 2-methyl-benzoxazole, and mono-chelator-functionalized 2-methyl-napthoxazole;

(b) a synthon selected from mono-chelator-functionalized 2,3,3-trimethyl-5-sulfanato-indole, mono-chelator-functionalized 2,3,3-trimethyl-6-sulfanato-benzindole, mono-chelator-functionalized 2-methyl-5-sulfanato-pyridine, mono-chelator-functionalized 2-methyl-6-sulfanato-benzothiazole, mono-chelator-functionalized 2-methyl-6-sulfanato-naphthothiazole, mono-chelator-functionalized 2-methyl-5-sulfanato-benzoxazole, and mono-chelator-functionalized 2-methyl-6-sulfanato-napthoxazole; and

(c) a synthon containing at least one carbon atom;
and then adding a transition metal.

72. The method of claim 71, wherein said coupling is performed as a single reaction step.

73. The method of claim 71, wherein said coupling comprises: either (i) first reacting (a) and (c) to form a product, followed by further reacting the product with (b); or (ii) first reacting (b) and (c) to form a product, followed by further reacting the product with (a).

74. The method of claim 71, wherein said chelator is protected during said coupling and deprotected thereafter.

75. The method of synthesis a compound of claim 1 by performing a Mannich reaction involving a xanthene, xanthanone, or phenoxazine detectable group, a secondary-amine derivative of a chelator, and formaldehyde; and then adding a transition metal.

744-37 PCT/US/CIP I

76. The method of claim 75, wherein said chelator is protected during said coupling and deprotected thereafter.

77. A kit comprising one or more containers, wherein at least one of said containers includes one or more molecules according to Formula (I).

78. A kit comprising one or more containers, wherein at least one of said containers comprises one or more molecules according to Formula (I), and one or more selected from the group consisting of:

- (a) one or more gels;
- (b) one or more containers including one or more molecules including a target sequence, said target sequence comprising an amino acid sequence of the form $(H)_i$, wherein H is histidine and i is an integer of from 4 to 12;
- (c) one or more containers including one or more antibodies having an epitope including an amino acid sequence of the form $(H)_i$, wherein H is histidine and i is an integer of from 4 to 12;
- (d) one or more containers including one or more denaturing agents;
- (e) one or more containers including one or more buffer; and
- (f) one or more sets of instructions.

79. The kit of claim 78, wherein said molecules according to Formula (I) are provided on at least one solid support.

80. The kit of claim 79, wherein said solid support is selected from the group consisting of a bead, a blot and a purification column.

744-37 PCT/US/CIP I

81. The kit of claim 78, wherein said one molecule according to Formula (I) is divalent.

82. A method for detecting one or more molecules that include a target sequence, wherein said target sequence comprises an amino acid sequence of the form (H)_i, wherein H is histidine and i is an integer of from 4 to 12, said method comprising:

- (a) providing a sample that comprises one or more target material, wherein said target material includes molecules having a target sequence,
- (b) subjecting said target material to electrophoresis in an electrophoretic medium;
- (c) contacting said electrophoretic medium with at least one molecule according to Formula (I) having a detectable group under conditions sufficient to permit transition-metal-chelate moieties of said molecule of Formula (I) to associate with said target sequence; and
- (d) detecting said detectable group, thereby detecting said one or more molecules that include a target sequence.

83. The method of claim 82, wherein said electrophoresis is selected from the group consisting of solution electrophoresis, SDS-PAGE, IEF, IPG electrophoresis, and 2D electrophoresis.

84. A composition comprising one or more molecules according to Formula (I) and one or more electrophoretic media.

85. The composition of claim 84, wherein said electrophoretic media comprises polyacrylamide.

744-37 PCT/US/CIP I

86. The composition of claim 84, further comprising one or more molecules including a target sequence, said target sequence comprising an amino acid sequence of the form $(H)_i$, wherein H is histidine and i is an integer of from 4 to 12.

87. A solution for staining target molecules in an electrophoretic medium, said solution comprising one or more molecules according to Formula (I), wherein said one or more molecules are present in a concentration sufficient to stain molecules including a target sequence in an electrophoretic medium, said target sequence comprising an amino acid sequence of the form $(H)_i$, wherein H is histidine and i is an integer of from 4 to 12.

88. A kit comprising one or more containers, wherein at least one of said containers comprises a stock solution of at least one molecule according to Formula (I).

89. A kit comprising one or more containers including the solution of claim 87.